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ANALYSIS OF THE MECHANISMS OF PLASTICITY AND FAILURE OF METAL OXIDE BASED NANOCERAMIC MATERIALS (REVIEW)

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Possible mechanisms of the plasticity and failure of nanoceramic materials based on ZrO_2 and Y_2O_3 and their mixtures are examined. It is established that macrodislocations — linear defects in the translational symmetry of a macrolattice whose sites are nanograins — are the most likely source of plastic deformation transfer in a nanocrystalline ceramics. In a continuum description of the mechanical properties of macrolattices it is correct to use models from the theory of dislocations and failure. Specifically, on this basis it is possible to describe mechanisms of plastic deformation and failure of nonceramic materials. The most likely reasons for the small excess plasticity of a nanoceramic are the high nonuniformity of the nanostructure and the substantial sizes of the pores after sintering. The most likely mechanism of failure is an increase in the size of the large pores, which is due to the emergence of a substantial number of macrodislocations on their surface.

Interest in using nanoceramics (NCERs) in different industries has been increasing in the last few years and the technologies for obtaining these materials are undergoing intense development [1, 2]. Their thermomechanical properties, specifically, the possibility of plastic deformation and resistance to failure during machining or use, largely determined the applications of NCERs. In this connection it is now timely to investigate the mechanisms of plastic deformation and failure of NCERs [1 – 20].

The study of the mechanical properties of NCERs is important not only from the applications and scientific viewpoints. Many experimental and theoretical works [2 – 10] have shown that the carriers of plastic deformation in the form of dislocations which are ordinarily present in polycrystals are virtually absent in the interior volume of nanocrystalline materials (NCMs) with average crystallite size not exceeding 20 – 50 nm. This means that the well-known dislocation mechanisms of plastic deformation and failure do not operate in such NCMs. Nonetheless, experiments with these materials show that under certain conditions they can deform not only in the plastic but also in superplastic regimes [11, 12]. Any attempt to explain these properties on the basis of the conventional theory of dislocations encounters certain difficulties [3 – 8].

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At the present time the description of the plastic behavior of NCMs and NCERs is based on a number of generally accepted models [1 – 9, 13 – 28]. To one extent or another, they are all based on the experimental observation that plastic deformation in polycrystals with ultrafine grains can occur by grain-boundary slip (GBS). The differences lie primarily in the mechanisms at the heart of this process. They can be divided conventionally into two groups. We shall place the mechanisms of global GBS in the first group (GBS1). Then the phenomena of grain-boundary slip encompass a substantial fraction of the intercrystallite boundaries and, on the whole, are distributed quite uniformly throughout the volume of the material [3, 4, 13 – 20]. We shall place the mechanisms of local GBS, where the macroscopic deformation of a NCM is represented as a combination of plastic shears which are strongly localized in relatively few planes lying between nanocrystallites, in the second group (GBS2) [5 – 8, 24 – 28].

At temperatures above the recrystallization temperature of the material, GBS1 deformation is observed experimentally in polycrystals with relatively large crystallites — $D > 100$ nm [13 – 17, 20]. As a rule, GBS2 processes develop for smaller crystallites $D < 100$ nm [7, 8, 11, 12].

The methods used for the microscopic description of the GBS mechanism differ by the choice of the type of structural defects and kinetic process which effectuate microplastic shear along grain boundaries.

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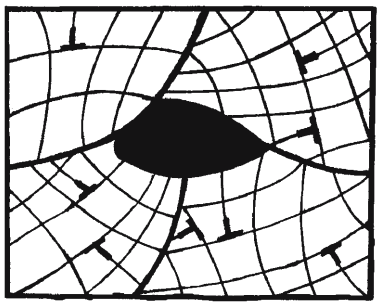

Fig. 1. Conventional scheme of the simplest hierarchy of nanograins in a metal oxide based ceramic: *thick lines*) boundaries of agglomerates consisting of nanograins; *solid black color*) pores located at the junctions of agglomerates; *thin lines*) intergrain boundaries separating nanocrystallites; ⊥) possible arrangement of macrodislocations inside an agglomerate (for clarity, nanograins are shown as quadrangles).

Some models explain GBS processes by the evolutionary characteristics of the dislocation subsystem of intergrain boundaries [1, 2, 17 – 20]. Often, grain boundary diffusion mass transfer or thermally activated migration of grains under an external load is used for the same purposes [1, 2, 13 – 17]. In a number of cases, model representations of nonequilibrium states of intergrain boundaries in strongly deformed polycrystals have been considered when analyzing this problem [17, 20]. In studies of the initial stages of the plastic deformation of a NCM, by analogy with the known processes of nucleation of a new phase during first-order phase transitions, thermal fluctuation nucleation of regions of microplastic shear has been analyzed [3, 4]. Models of volume diffusion – viscous flow of polycrystalline bodies which is accompanied by GBS processes have also been constructed [29]. A feature that these methods have in common is that they are all primarily designed to describe GBS1 processes.

Methods for simulating the plastic deformation of NCMs, based on relatively new ideas about macroscopic defects in the polycrystalline structure of materials, have been undergoing intensive development in the last few years. These works originated in the analysis of topological defects which represent a breakdown of the translational symmetry of a regular, periodic, macrolattice whose sites are polycrystallites [21 – 23]. Different variants of microscopic models of topological defects are presented in many works: superdislocations — for submicrocrystalline polycrystals [24, 25]; macrodislocations — for describing linear defects in the translational symmetry of arbitrary macrolattices [5 – 8, 26, 27]; nanodefects — for macrolattices whose sites are occupied by nanocrystallites [28]; and, so forth. Following [5 – 8, 26, 27], for brevity, we shall employ the most general term for a linear topological defect in a macrolattice — a macrodislocation.

Since macrolattices possess the obvious property of anisotropy and macrodislocations have completely determined slip planes, these models could be helpful in explaining the effects due to localization of plastic shear.

Our objective in the present article is to provide experimental and theoretical validation for using the existing models of macroscopic dislocation-type linear defects in polycrytalline materials to analyze the mechanisms of plastic deformation and failure of a metal oxide based nanoceramic material.

We used atomic forms microscopy (AFM) and x-ray structural analysis to investigate fractures produced at room temperature during mechanical impact bending tests on samples of a Y_2O_3-doped ZrO_2 nanostructured ceramic. The samples were made by dry pressing of nanostructured powders, which were exposed to ultrasound at the same time, followed by sintering. The ultrasonic power was varied over a wide range [30, 31]. The particles of the initial powder were flat, 20 – 30 nm thick, disks with an average diameter of about 150 nm. The structure of the particles consisted of nanograins with an average diameter of about 25 nm.

A complicated hierarchy of nanograins was obtained in some processing regimes. Figure 1 shows a complicated scheme of one such nanostructure. A NCER as a whole is an agglomerate consisting of single-phase monolithic formations (aggregates) which are sintered together with pores of various sizes present at the junctions. A nanostructure, partially inherited from the initial material, is present inside the aggregates. The average size of the aggregates is ordinarily 1 – 10 μm. In some cases, aggregates can consist of subaggregates. Then, the subaggregates inherit the nanostructure of the initial powder. More complicated nanograin hierarchies are possible in multiphase NCERs [30, 31].

Figure 2 shows an AFM image of the fracture surface of a ZrO_2 nanostructural ceramic, obtained by compaction under pressure 150 MPa using ultrasound with power 1 kW. The AFM measurements were performed in a semicontact mode on a freshly cleaved surface of samples using a P47-MDT (NT-MDT, Zelenograd) scanning probe microscope. Aggregates and a large pore located between them can be seen clearly in the image. Planes of localized plastic shear, which divide the body of the aggregates, can be clearly seen. Data obtained in a synchronous study in the phase-contrast regime and clearly showing the grain structure of the aggregates as well as topological measurements which permit making a quantitative evaluation of the parameters of the surface relief greatly supplement the AFM observations.

The data presented in Fig. 2 and the results of an x-ray structural determination of the sizes of the regions of coherent scattering show that the initial nanostructure is not inherited completely. As the pressed objects are sintered, a primary nanograin partially recrystallizes. Since during pressing many nanograins are under different stresses and in different deformed states, recrystallization gives rise to appreciable variance in the sizes and shapes of nanograins. At the junctions of aggregates adjoining the surface of primary pores the deformation of nanograins is minimal and therefore

here their size should be close to that of the initial nanograin. The measurements performed at these locations (see Fig. 2) show that the size of the nanocrystallites is close to 20 – 30 nm.

Characteristically, staircase steps form on the fracture surfaces of NCERs (see Fig. 2*a*). The step sizes are multiples of the nanocrystallite sizes (see Fig. 2*b* and *c*). Similar steps have been observed experimentally in studies of fractures breaks of the same NCER by electron microscopy [30] and in AFM studies of the surface topography of mechanically activated metal powders with a similar nanostructure [7, 8, 26, 27].

Observations of the effects due to the localization of plastic shear performed with an electron microscope [11, 12] agree well with the general picture of localized plastic flow of aggregates which was obtained by AFM methods. It is seen clearly in Fig. 2*a* that the staircase steps are sites where localized plastic shear planes emerge at a free fracture surface. However, the mechanism of the relative displacement of neighboring nanocrystalline planes of the macrolattice and the reasons why the height and length of the staircase steps are multiples of the nanograin size remain unexplained.

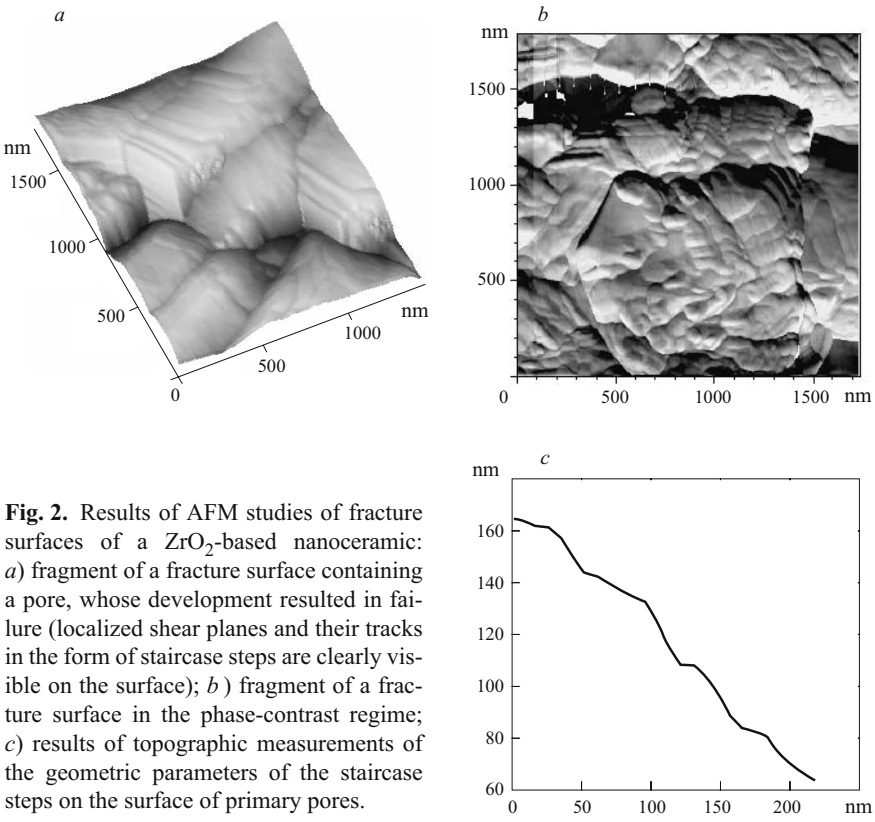

Fig. 2. Results of AFM studies of fracture surfaces of a ZrO_2-based nanoceramic: *a*) fragment of a fracture surface containing a pore, whose development resulted in failure (localized shear planes and their tracks in the form of staircase steps are clearly visible on the surface); *b*) fragment of a fracture surface in the phase-contrast regime; *c*) results of topographic measurements of the geometric parameters of the staircase steps on the surface of primary pores.

The steps and plastic shear localization planes in NCERs are very similar to the tracks of slip planes of edge dislocations arising in the interior volume and on the surface during plastic deformation of ordinary (not nanocrystalline) metals.

It can be hypothesized that the tracks are left by macroscopic dislocation-type linear defects determined on macrolattices (Fig. 3*a* and *b*). Many investigators have observed such defects experimentally [21 – 23, 28]. It is evident that some of them are formed during synthesis of a nanocrystalline state and some arise directly during plastic deformation. They could appear as a result of, for example, thermal fluctuation nucleation of regions of microplastic shear during deformation [3, 4] or thermally activated migration of grains under stress [13, 16, 17, 20].

This hypothesis also offers a simple explanation for the observed facts that plastic shear is localized along intergrain planes and the sizes of the steps where these planes emerge on fracture surfaces are multiples. Indeed, in this case the plastic shear localization planes are simply the slip planes of macrodislocations, and when they emerge onto a fracture surface edge dislocations can leave steps whose sizes must be multiples of their Burgers vector.

There are many models of the macrodislocations which elaborate the structure of the cores of the dislocations, the mechanisms of their movement, and so forth to one degree or another [5 – 8, 24 – 28]. Consequently, the problem is to choose from among these models the one that would most fully take account of the salient aspects of the deformation and failure of NCERs under real working conditions. The well-known models are briefly analyzed below.

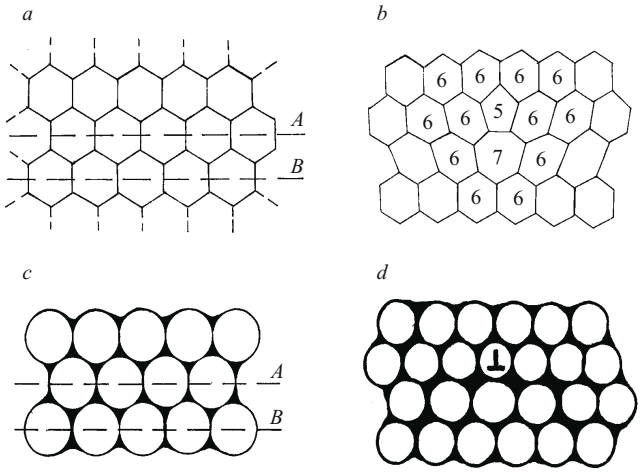

Fig. 3. Models of topological defects in a polycrystalline structure: *a*) planar section of a regular, periodic, close-packed macrolattice whose sites are occupied by identical polycrystals; *b*) topological defect in the translational symmetry, containing a breakdown of the regular faceting (the integers denote the number of polycrystallite faces in the cross-sectional plane); *c*) mechanical structure of a macrolattice with a fluid-like grain-boundary medium and rigid spherical kernels of polycrystals; *d*) mechanical structure of the core of a macrodislocation [5].

If a NCER were to consist of nanograins of the same shape and size, regularly arranged and close-packed in a periodic space lattice, then in a planar section it could have the structure shown in Fig. 3*a*. For crystallites no larger than 20 – 30 nm, the central part of a grain body will be rigid and incapable of plastic deformation under real loading conditions. In order for such a structure as a whole to be capable of plastic deformation with the shape of the nanograins remaining unchanged, grain boundary slip on the intergrain boundaries must be possible. But an ideal periodic structure even in this case will exert a substantial resistance to plastic shear. To see this, it is sufficient to take account of the fact that for a localized displacement of one plane *A* of nanocrystallites relative to another plane *B* (see Fig. 3*a*) work must be done to overcome the grain-boundary friction forces. The magnitude of these forces is proportional to the areas of the displaced surfaces, and the specific friction force during grain-boundary shear is, as a rule, quite large.

If the nanostructure contains a topological defect such as the one shown in Fig. 3*b*, then plastic deformation of the material can be facilitated. In this case grain-boundary shear occurs not along the entire plane at once but only between neighboring nanograins in the core of a defect. The area occupied by the core is, evidently, always less than the area of the shear surfaces *A* or *B* (see Fig. 3*a*). Therefore, one such defect is always more easily shifted than the entire plane.

The most noticeable differences between the currently existing models of macrodislocations are in the description of the dislocation mobility [5 – 8, 24 – 28]. The mobility is due to the corresponding mechanisms of macrodefect movement under applied external stresses.

The mathematical model proposed in [24, 25] for a superdislocation is based on the assumption that a superdislocation is a pile-up of infinitely long, parallel, rectilinear grain-boundary dislocations. This links the mobility of a superdislocation to the possibility of conservative motion of dislocation pile-up along intergrain boundaries. However, in the first place, unbounded rectilinear dislocations or dislocation pile-ups, lying in a single plane passing along intergrain boundaries, simply do not exist in polycrystalline structures. In the second place, it is known that purely conservative motion of a network of real grain-boundary dislocations is impossible [3, 4, 16, 17, 20 – 23].

A number of the models examined in the review in [28] have similar drawbacks. The scheme of macrodislocations with an integral Burgers vector presented in this work (in the article they are designated by the somewhat unfortunate term "nanodefects," tying their existence solely to nanostructures) is completely identical to the topological defect shown in Fig. 3*b*. As a generalization, some models of partial macrodislocations and stacking faults in a macrolattice are also examined there. The mobility of macroscopic defects in these models is due to slip and climb of pile-ups of grain-boundary and near-boundary dislocations. Their strong interaction with the junctions of grains and extremely low density are ignored. The work does not contain any mathematical model that would serve to evaluate the mobility of macrodefects. As a result, using these models it is difficult of evaluate the stresses of plastic flow and failure in NCERs.

The experiment performed in [11] provides a real foundation for correctly choosing a macrodislocation model. In this experiment the conditions for increasing the plasticity of zirconium oxide based ceramics and the possibility that these ceramics can transition into a superplastic state, depending on the amount of other chemical components added, was investigated. Specifically, it was shown that additives that intensify the activity of grain-boundary diffusion increase the plasticity of the material and facilitate a transition of the material into a superplastic state. In their presence superplasticity appeared at lower temperatures and with high deformation rates. This shows that the deformation properties of NCERs can be described most accurately using models where diffusion mass transfer along grain boundaries and junctions plays the main role in the motion of macrodislocations.

One possible model of this kind was proposed in [5] and extensively used in [6 – 8, 26, 27] for theoretical interpretation of a number of experimental facts, observed in the nanostructures of metals and amorphous cluster materials. The salient features of this model are as follows.

It is assumed that nanocrystallites forming a macrolattice (see Fig. 3*a*) have a nonuniform mechanical structure. The central part (shown in Fig. 3*c* as spheres) is rigid. The peripheral region is a thin layer, one or two lattice parameters thick, which consists of fluid-like medium moving by diffusion (colored black in Fig. 3*c*). This medium contains the entire cellular structure of the grain-boundary dislocations and grain junctions as well as segregated impurity elements, point defects, and so forth. On the whole its motion is considered to be viscous flow. When the nanomaterial is deformed, the grain-boundary medium can flow between the spheres, similarly to a liquid in porous substances. Such kinetic similarity to real liquid media is not a consequence of its structural similarity to a liquid phase. It is merely a manifestation of the quite high values of the grain-boundary diffusion coefficients and diffusion along grains junctions, since even in real liquids viscous flow in thin layers of molecular size occurs only by means of diffusion mass transfer.

It is known that the volume diffusion in solids starts to play an active role in structure formation at temperatures equal to or higher than the recrystallization temperature T_r. For chemically pure materials $T_r \approx (0.3 – 0.4)T_{melt}$ (T_{melt} is the melting temperature of the material) and for materials containing impurities $T_r \approx (0.4 – 0.5)T_{melt}$ [32, 33]. The activation energy of grain-boundary diffusion is on average approximately half the activation energy of volume diffusion [32, 33]. This means that the characteristic activation temperature T_s of grain-boundary diffusion is approximately half the recrystallization temperature. For example, for carbon

steels $T_{melt} \approx 1600 - 1700$ K and $T_r \approx 600 - 800$ K. Therefore, $T_s \approx 300 - 400$ K. For NCERs $T_{melt} \approx 2000 - 2500$ K and $T_s \approx 400 - 600$ K. Hence, grain-boundary diffusion of impurities in many materials can remain active at temperatures only slightly above room temperature.

In turn, the activation energy of diffusion along the grain junctions is even lower (according to different data it is $1/3 - 1/4$ times the activation energy of volume diffusion) [32]. Consequently, the temperature threshold T_{min} for diffusion along the grain junctions should be less than T_s. Estimates for NCERs give $T_{min} \approx 200 - 400$ K.

We also call attention to the following important circumstance that gives rise to diffusion at low temperatures. It is evident from the diagram in Fig. 3*d* that macrodislocations move by local intergrain slip of spheres which comprise the core of a macrodislocation. It is due to viscous diffusion flow of the near-boundary medium over very short distances, comparable in size to nanocrystals. Therefore, other conditions being equal, the shorter this size, the more effective diffusion mass transfer and the more mobile macrodislocations are.

Thus, even at quite low temperatures, close to T_{min}, diffusion can occur actively in the core of a macrodislocation of NCMs and NCERs and give rise to macrodefect mobility. This means that the model proposed in [5] for a macrodislocation is applicable not only in the high-temperature range ($T > T_r$). There is every reason to use it for simulating plastic deformation of NCMs and NCERs in a much wider temperature range $T \geq T_{min}$.

We shall use a continuum description of models of plastic deformation and failure of NCERs. The deformation and stress field generated by macrodislocations can be easily calculated in the continuum approximation similarly to the manner in which this is done in the continuum theory of dislocations [21, 23]. Indeed, following the standard prescription for switching to the continuum description of space lattices, we replace a macrolattice consisting of nanocrystallites by an effective continuous medium with macroscopic shear modulus G and Poisson ratio ν [5, 21, 23]. It can be assumed that the material point in such a medium is larger than a nanocrystallite.

The model of an edge dislocation in a continuous medium consists of an extra half-plane of thickness h inserted into a corresponding section of the initially unstressed material. The value of h is not regulated in any way, since in a continuous medium there are no characteristic length scales [21 – 23]. As a rule, these scales are introduced into the theory from outside the theory taking account of the real dimensions of physical objects described in this approximation. For example, in the continuum theory of dislocations of an atomic crystal lattice it is ordinarily assumed that h is comparable to the lattice parameter a. If h is equated to the parameter of an atomic crystal lattice we obtain a model of an ordinary lattice edge dislocation with an integral Burgers vector [21 – 23]. However, if h is set equal to the periodicity parameter of a macrolattice $b = D$, we obtain a continuum model of an edge macrodislocation, likewise with an integral Burgers vector b [5, 28]. In this case, there are no violations of the rules for a transition to a continuum description of a medium with defects either from the microlevel (as in the case of an atomic lattice) or from the macrolevel (when this method is applied to macrolattices). This is the point of the well-known universality of the methods of the mechanics of continuous media and the thermodynamics of a deformable solid body [5, 21 – 23, 28, 29, 32 – 36].

It is also obvious that the mathematical description of the defects in an atomic lattice as well as in a macrolattice in a continuum theory with be identical until the structure of the sites of the corresponding lattices changes under a deformation. In atomic lattices this condition is always satisfied automatically as a result of the assumed rigidity of the atoms. In a macrolattice such an approach is possible if the deformation of the material in a macrodislocation core does not lead to substantial plastic distortions of the spherical shape of the spheres. This requirement supposes that only continuum models in which the stress and strain fields do not diverge at the core of a linear defect are used. The well-known Peierls – Nabaro model, which is often used in the continuum approximation to remove divergences of this kind, satisfies this condition [5, 23]. For these reasons the Peierls – Nabaro model was also used in [24, 25] to construct a model of a superdislocation.

Using this model it is possible to evaluate the stresses required to overcome the Peierls barrier in a macrolattice of nanocrystallites [5]:

$$\sigma_P = \frac{2G_1}{(1-\nu)} e^{-\frac{4\pi\xi}{b}}, \qquad (1)$$

where $b = 2R$ is the Burgers vector of the macrodislocation (R is the average radius of a crystallite); $2\xi \sim b$ is the width of the macrodislocation; G_1 is the modulus of local shear of the medium [5]:

$$G_1 = \frac{1}{3}\left\{K_1\left[\frac{R}{V_l}\left[R + 4\sqrt{\frac{RK_f\rho}{3\gamma_l\eta v_d}}\right]^{-1} - V_l\right] - K_s V_s\right\}, \qquad (2)$$

where V_l is the volume fraction of the viscous fluid-like phase of the grain-boundary material; V_s is the volume fraction of the solid phase; K_1 and K_s are the bulk moduli of these phases; $\gamma_1 = 1/K_1$ is the compressibility of the grain-boundary phase; K_f, η, and ρ are, respectively, the coefficient of filtration in the macrolattice, viscosity, and density of the grain-boundary material; and, v_d is the velocity of the macrodislocation.

In thin molecular layers, viscous flow of the material between the spheres is possible only by means of diffusion. In this case

$$\left.\begin{aligned} \frac{K_f}{\eta} &= \frac{\Omega D_e}{kT}\frac{3\delta}{2R}; \\ V_l &\approx \frac{3\delta}{2R}, \end{aligned}\right\} \tag{3}$$

where Ω is the atomic volume of the material diffusing along a grain boundary; D_e is the effective diffusion coefficient, which includes the diffusion along the grain boundaries and junctions; δ is the diffusion thickness of the boundary; and, k is Boltzmann's constant.

Setting $K_1 = K_s = K$ for simplicity, and using the relation $V_s + V_l = 1$ and Eq. (3) we obtain for G_1 the expression

$$G_1 = \frac{K}{3}\left\{\frac{2R^2}{3\delta}\left[R + 4\sqrt{\frac{D\Omega\rho K\delta}{2kTv_d}}\right]^{-1} - 1\right\}, \tag{4}$$

It follows from Eqs. (1) – (4) that as the nanocrystallite sizes and (or) the plastic deformation rate decrease the shear modulus G_1 and the Peierls barrier go to zero. This means that conditions of plastic deformation under which the deformation of the polycrystallites in a macrodislocation core will be small and therefore the continuum description of the fields generated by a macrodislocation will be correct can always be foundt. It can be shown that for nanostructures with crystallites no larger than 50 – 100 nm these conditions are satisfied for essentially all stress and strain regimes used in practice [7]. We also note that sufficiently low Peierls barriers can lead to a transition of NCERs and NCMs into a superplastic state.

The analogy between the continuum description of dislocations and macrodislocations can be extended to a description of macrodislocation mechanisms of plastic deformation and failure of NCERs. Indeed, according to the continuum theory, replacing a nanoceramic macrolattice with an ensemble of macrodislocations of an effective continuous medium, we obtain a model of a continuous solid body with linear defects that is identical to the model obtained on switching from a continuum description of an atomic crystal lattice with dislocations. This follows from the fact that in a continuous medium there are no intrinsic length scales that would make it possible to distinguish one model from another without leaving the framework of the continuum analysis. But then, when studying the mechanical behavior of NCMs, practically all known models and the corresponding methods of describing plastic deformation and fracture of materials such that no divergences occur in the stress and strain fields can be taken over completely from the continuum theory of dislocations [21, 23, 24].

In such an approach the process of plastic deformation of nanomaterials is represented as a motion of an ensemble of macrodislocations in the volume of the body (see Fig. 1), in complete agreement with the manner in which the plastic deformation of a crystal lattice is represented as a motion of an ensemble of dislocations. The plastic deformation rate $\dot{\varepsilon}$ in this case is expressed in terms of the average velocity and density ρ_{md} of macrodislocations according to the expression

$$v_d = \frac{\dot{\varepsilon}}{b\rho_{md}}.$$

Just as in the analysis of ordinary dislocations, we assume that various kinds of obstacles can also impede the motion of macrodisocations. In NCERs such obstacles could be the boundaries of agglomerates which are analogues of intercrystallite and interphase boundaries in polycrystalline alloys, inclusions of foreign phases, nonuniformities whose sizes are close to those of nanograins, serving as analogues of different atoms on crystal lattices, and so on (see Fig. 1). Then, macrodislocation pile-ups, which act as stress concentrators near which primary foci of failure in an initially continuous medium can appear, can form on these obstacles under certain conditions [21, 23, 34]. The mathematical description of such processes within the continuum theory will also remain the same as before.

If a NCER contains ready continuity defects in the form of quite large macropores (see Fig. 1), these pores can easily become initial foci of failure. This requires that a pore become a rigid stopper for a macrodislocation pile-up. Then, under external stresses some segments of a macrodislocation pile-up will vanish in the pore, correspondingly increasing its volume and changing its shape. Processes of this kind are well known and widely used to describe within the framework of a continuous medium the failures of a crystal lattice. In so doing, it is assumed that they lead to a transformation of embryonic microcracks and pores into macroscopic cracks [21, 23, 34]. Considering the well-known universality of the continuum description of the mechanical properties of materials, we point out that there are no grounds for not using these models of failure to examine the corresponding phenomena in NCs.

The transition to the continuum approximation makes it possible to assess the degree to which small pores participate in failure processes in NCERs according to the macrodislocation mechanism described above. If a pore has the size of a nanocrystallite, then it is a vacant site of a macrolattice — a macrovacancy. In the continuum approximation its size is less than that of a material point in an effective continuous medium. Since Burgers vector of a macrodislocation is comparable to the size of a pore, in a macrolattice these defects will interact with one another approximately just like ordinary dislocations interact with atomic vacancies, i.e., macrodislocations can entrain a pore and drag it through the volume of a nanostructured material.

This can be explained in a natural manner in the continuum approximation, where it is always assumed that the motion of a dislocation gives rise to motion of the material points of the medium and with them macrovacancies also.

Therefore, such a pore is not an efficient stopper for macrodislocations and its presence in the material cannot create the conditions for development of failure foci. This suggests that the real foci of possible failure of nanomaterials by the macrodislocation mechanism must be pores containing a quite large number of vacant macrosites.

Since the movement of large pores as a whole requires the expenditure of large amounts of energy, on the one hand these pores can become effective stoppers for macrodislocation pile-ups and on the other hand they are an initial continuity defect which is capable of growing without bound. A pore which initiated the growth of a microcrack at the observation site is shown in Fig. 2*a*. It is evident that the pore is much larger than not only the steps from the points of emergence of dislocations but also all agglomerates neighboring it.

The proposed continuum description of the mechanisms of plastic deformation and failure of macrolattices is physically close to the well-known method of investigating complex hierarchical structures as multilevel systems [35, 36]. The multilevel description presumes that not only a microlevel but also meso- and macrolevels in real thermodynamic systems can have defects in their own structure which have a definite effect on the mechanical properties of a material. In this connection the boundaries of aggregates, large pores, and macrodislocations in NCERs should be seen as structural defects at the macrolevel, where the main processes of plastic deformation of a material as a whole develop. Then, the intergrain medium and the rigid spherical kernel of a nanocrystallite must be put into the mesolevel. The microlevel structure of the intergrain medium consists of segments of grain-boundary dislocations lying in the planar facets of nanocrystallites, grain junctions, near-boundary volume dislocations, and various kinds of point defects (vacancies, interstitial and impurity atoms).

According to [35, 36] macrodefect kinetics govern macrolevel deformation processes. The dynamical characteristics of macrodefects are determined by the structure and kinetic properties of the medium at the mesolevel, and in turn they depend entirely on the structure and diffusion mobility of objects at the microlevel. Thus, the proposed approach to describing the mechanical properties of NCERs is, essentially, one variant of the well-known multilevel method [35, 36].

In summary, macrodislocations — linear defects of the translational symmetry of a macrolattice whose sites are nanograins — are the most likely carriers of plastic deformation in nanocrystalline ceramics.

In the continuum description of the mechanical properties of macrolattices it is correct to use models of the theory of dislocations and failure which do not contain divergences of the stress and strain fields. Specifically, the mechanisms of plastic deformation and failure of nanoceramic materials can be described on this basis.

The small excess of plasticity (brittleness) of NCERs is probably due to the high nonuniformity of the nanostructure and the substantial pore sizes after sintering.

The most likely mechanism of failure is growth of large pores which is induced by the emergence of a substantial number of macrodislocations onto their surface.

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